Extracting useful information from noisy exponentially decaying signals

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Analysing data that consists of one or more truncated exponential functions is of great interest in a wide range of fields. Data consisting of one or more exponential functions are measured by a wide range of instruments, examples include: nuclear magnetic resonance, (NMR); magnetic resonance imaging (MRI); the analysis of radioactive decay data; chromatography; lifetime fluorescence imaging; spin resonance, (ESR). Many of the algorithms that are currently in used for 'characterising' this data, are difficult to interpret or are they useless and they produce erroneous results. Some of the key technical issues associated with this problem are discussed in this article we also present some results that use some elementary properties of exponential properties of exponential and harmonic functions. These properties allow us to develop relationships between these functions which we exploit to analyse exponentially decaying signals in noisy environments.

Introduction

In this article we derive a simple technique for analysing and characterising data consisting of one or more truncated exponential functions. We exploit a number of simple mathematical relationships between these functions and the harmonic functions, $\cos(x)$, and $\sin(x)$. We use these relationships to derive expressions that enable us to characterise truncated exponential signals from single exponential functions in noisy environments. This approach can be generalised to characterise data from signals consisting of more than one exponential function in a noisy environment. Many physical phenomena are described by systems of one or more differential equations. The solutions of these systems will in general consist of one or more exponentially decaying functions. In order to use the data generated by these systems to determine their physical characteristics it would be useful to have a robust mathematical technique that could determine the decay constants and amplitudes of each of the exponentially decaying component signals that occur in a set of measurements. In particular it would be useful to be able characterise truncated exponential signals.

Signals consisting of one or more exponential functions arise in a number of areas, examples include: deep level transient spectroscopy, in semiconductor physics, Istratov and Vyvenko (1999); fluorescence decay analysis in the analysis of biological samples Jones et al (1999); the analysis and characterisation of time series measurements from radioactive samples, Cottingham and Greenwood, (2001); the analysis of the relaxation phenomena that occur in nuclear magnetic resonance studies of materials, Cowan, (1997); reaction kinetics, Érdi and Tóth, (1989); positron emission tomography, Valk et al (2003); MRI, Wells (1982), the Biacore, Fersht (1999).

Attempts at doing a least squared fit of one or more exponentials to data and varying the decay constant(s) and the amplitude(s) to get a best fitting exponential function are fraught with algorithmic difficulties. The results are often misleading and ambiguous, even when the noise level in the data is low. These approaches are still unfortunately in wide use. Some authors seem to be unaware of the technical problems that are associated with processing data that consists of one or more exponential functions, e.g. Baxter et al (1994) and (1995), Lubic (2001), Valk (2003). The algorithmic problems associated with attempting to fit exponential functions to data have been discussed by a number of authors e.g. Sivia (1996), Gans (1992), Istratov and Vyvenko (1999), Fersht (1999), Acton (1990).

The approach that we are suggesting in this article should help to provide a mathematical basis for choosing the points in time at which data can be collected; should provide a means of analysing and characterising truncated exponential signals, this is a major technical problem as people that analyse data that contains even a single exponential tend to wait till the signal is close to its zero level before attempting to characterise the signal, Cowan (1997); the technique also provides a link between harmonic functions and exponential functions, that can still be of value when noise is present; in principle it should be possible to generalise this work in order to analyse data consisting of more than one exponential function. Making the link between exponential and harmonic functions may enable us to develop ways of improving on the resolution arguments that were given by Istratov and Vyvenko, (1999), for analysing data consisting of a number of exponentially decaying signals.

Mathematical Analysis

The techniques that we develop in this article are concerned with the analysis and characterisation of data of the form

$$f(t) = \sum_{j=1}^{\infty} C_j e^{-\lambda_j t} + n(t) \tag{1}$$

The noise is expressed by the term n(t). This term or function can be thought of as a stochastic function of the time. We begin the analysis by utilising some properties of Chebyshev polynomials.
The Chebyshev expansion of an exponential function has the form

$$e^{-\alpha x} = 2I_0(\alpha)T_0(\alpha x) + 2\sum_{j=1}^{\infty} T_j(\alpha_k x)I_j(\alpha)(-1)^j \tag{2}$$

Arfken and Weber, (2000) where I_m represents modified Bessels functions of order m. The Chebyshev expansion occurs over an interval, $-1 \leq x \leq 1$. In practice when data has been collected over an interval such that $x_{min} \leq x \leq x_{max}$, this interval can be converted to the interval $-1 \leq \overline{x} \leq 1$, by using the transformation

$$\overline{x} = \frac{2x - x_{min} - x_{max}}{x_{max} - x_{min}} \tag{3}$$

Thus the Chebyshev expansion for an exponential function can be generalised to an exponential function that is defined over a general finite interval, e.g. $-1 \leq x \leq 1$.
Consider a signal, $f(t)$, consisting of an exponential function and some noise, where

$$f(t) = Ce^{-\lambda t} + n(t) \tag{4}$$

$f(t)$, can be expressed as a series of Chebyshev polynomials, where

$$f(t) = \sum_{n=0}^{\infty} A_n T_n(x) \tag{5}$$

In practice the sum will of course be done over a finite number of terms, and so the function f(t) will be represented by an approximation of the form

$$f(t) \approx \sum_{n=0}^{N_{max}} A_n T_n(x) \tag{6}$$

where N_{max} is the highest order term used in the Chebyshev expansion for $f(t)$. This process facilitates the reduction of noise. Noise reduction is achieved by expanding the data in terms of Chebyshev polynomials and discarding all of the terms above a particular order. The value of N_{max} can be estimated or decided upon by the user. For example this could be acheived by prior experimentation on a time series containing exponential functions and some computer generated pseudo random noise with the characteristics that are likely to be generated by the equipment that measures the signal of interest.

Relating a series of exponential functions in a noisy environment to a series of harmonic functions in a noisy environment can be acheived by converting a series of Chebyshev polynomials, $T_n(x)$, to a power series in x. Chebyshev polynomials can be defined by the the following expressions

$$T_0(x) = 1 \tag{7}$$

$$T_1(x) = x \tag{8}$$

and the recursion relation

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \tag{9}$$

Fox and Parker, (1968).
Consider an exponential function, this can be expressed in terms of a power series

$$e^{ax} = \sum_{n=0}^{\infty} \frac{(ax)^n}{n!} \tag{10}$$

This can of course be approximated by

$$e^{ax} \approx \sum_{n=0}^{N_{max}} \frac{(ax)^n}{n!} \tag{11}$$

where the N_{max}th order term i.e. $x^{N_{max}}$, is the highest order term that is used in the approximation. The expansion for $\sin(ax)$, is given by

$$\sin ax = \sum_{n=0}^{\infty} \frac{(-1)^n (ax)^{2n+1}}{(2n+1)!} \tag{12}$$

This can be approximated by

$$\sin ax \approx \sum_{n=0}^{N_{max}} \frac{(-1)^n (ax)^{2n+1}}{(2n+1)!} \tag{13}$$

similarly the expansion for $\cos(ax)$ is given by

$$\cos ax = \sum_{n=0}^{\infty} \frac{(-1)^n (ax)^{2n}}{(2n)!} \tag{14}$$

The algorithm involves expanding the exponential in terms of some polynomials or splines, e.g. Chebyshev polynomials. The odd order terms are separated from the even order terms. The odd Chebyshev polynomials are then expanded out into a set of terms that consist of powers of x.
Similarly the even terms can also be expanded into a power series. One way of converting the power series of an exponentially decaying signal where noise is not present to a power series for cosine and sine functions is to multiply all of the negative terms in the power series that is obtained for e^{-ax} by -1, i.e. terms of the form x^r, are multiplied by -1. This yields the power series for, e^{ax}. Now consider the odd order terms in the power series, terms where the power in, x^r, satisfies, $r = 2q + 1$.
If $\frac{r-1}{2}$, is even or equal to zero, the term is left untouched. If $\frac{r-1}{2}$, is odd the term is multiplied by -1. This yields the power series for $\sin(ax)$.

Consider the even order terms in the power series. If $\frac{r}{2}$, is even or equal to zero, the term is left untouched. If $\frac{r}{2}$, is odd the term is multiplied by -1. This yields the power series for $\cos(ax)$.
Thus the even powers of the expansion of the function, $f(x) = e^{ax}$, when processed as above will yield the function $\cos(ax)$.

This process can be thought of in terms of obtaining a power series in x and then replacing x by the imaginary number $z = ix$, where $i = \sqrt{-1}$. Thus

$$e^{x} \rightarrow e^{ix} \equiv \cos(x) + i\sin(x) \tag{15}$$

The harmonic functions that are generated from the exponenentially decaying (growing) signals can of course be processed by a range of standard techniques such as Fourier based techniques, such as the fast Fourier transform. In practice it is likely that the user will only have a small section of the harmonic signal, that spans less than a full periodic cycle of the harmonic functions that are generated by the above process. One way of overcoming this is to multiply the expansions for $\cos(ax)$ and $\sin(ax)$by a suitable harmonic function and then to recombine them. Consider the following trigonometric relationship

$$s(x) = \cos(\alpha x)\cos(\Omega x) - \sin(\alpha x)\sin(\Omega x) \equiv \cos(\Omega x + \alpha x) \tag{16}$$

This is generated by multiplying the term $\cos(\alpha x)$, by $\cos(\Omega x)$, and the term, $\sin(\alpha x)$, by $\sin(\Omega x)$, If Ω, is chosen so that it varies by at least one cycle over the interval in which the power series approximations for $\sin(\alpha x)$ and $\cos(\alpha x)$ were generated, it should result in there being more than one cycle of the function s(x) over the interval of the variable x in which we have generated approximate power series for, $e^{\alpha x}$, $\cos(\alpha x)$ and $\sin(\alpha x)$. A number of other harmonic functions can be generated from the power series for $\cos(\alpha x)$ and $\sin(\alpha x)$, with the aid of the standard trigonometric identities, e.g.

$$\sin([\Omega \pm \alpha]x) \equiv \sin(\Omega x)\cos(\alpha x) \pm \cos(\Omega)\sin(\alpha x) \tag{17}$$

and

$$\cos([\Omega \mp \alpha]x) \equiv \cos(\Omega x)\cos(\alpha x) \pm \sin(\Omega)\sin(\alpha x) \tag{18}$$

If Ω is chosen appropriately this process results in the generation of one or more cycles of a harmonic function.

The functions $\sin([\Omega{\pm}\alpha]x)$ and $\cos([\Omega{\pm}\alpha]x)$can then be analysed by using a suitable harmonic analysis technique e.g. the periodogram or a fast Fourier transform. If data is collected over a number of closely spaced data points this will tend to benefit the harmonic frequency analysis of the periodic function that is generated from the exponential. This process can be generalised to a range of data intervals, e.g. in practice a user may not wish to set the origin in the middle of some interval of the dependent variable. It may be more advantageous to obtain an approximation for the exponential function and subsequently the sine and cosine functions by expanding a point other than $t = 0$.

Some results

Consider a signal that consists of a single exponential function, $e^{-\lambda x}$, where the noise term is equal to zero. If the data is collected between the points $t = 0$ and $t = t_{max}$, this can be rescaled to $\frac{-t_{max}}{2} \leq t' \leq \frac{t_{max}}{2}$, using equation (3), we can define a new variable $\overline{x}$, where $-1 \leq \overline{x} \leq 1$. The data will be collected at a finite number of data points in this interval, note the points do not need to be evenly spaced. A Chebyshev expansion can be obtained for this signal using software such as the NAG subroutine E02ADF. The Chebyshev expansion can be use to generate a power series expansion in terms of the variable $\overline{x}$. From the arguments presented above this can be converted into two power series, one for $\sin(\lambda x)$, and one for $\cos(\lambda x)$. The cosine series is generated from the even order terms, i.e. terms of order, $0, 2, 4, \cdots$, and the sine series from the order terms, i.e. terms of order, $1, 3, 5, \cdots$. The above approach works well in the zero noise case. Some results for the noise free case are presented in figure (1a), figure (1b), figure (1c) and figure (1d). In figure (1a) a plot of an exponential composed of twenty five equally spaced data points is presented. The corresponding sinsuoid and cosinusoid are presented in figures (1b) and (1c). In figure (1d) a plot based on expression (16) is presented, the angular frequency corresponding to $\Omega + \alpha$, is 23.56 s^{-1}. In these figures, $t_{min} \leq t \leq t_{max}$, where, $t_{max} = 1s$, $t_{min} = -1s$, and thus the variable $\overline{x}$, is equivalent to the variable, t.

Some plots for a simulated data set consisting of 250 evenly spaced and normally distribiuted noise with a standard deviation of: 1×10^{-2} units, 1×10^{-1} units, and 5×10^{-1} units, are presented in figures (2), (3) and (4) respectively, in all of the cases the mean of the noise is 0.0 (units) and the angular frequency corresponding to $\Omega + \alpha$, is 23.56 s^{-1}. These plots illustrate

the possibility of extracting a harmonic signal from a noisy exponential even when the noise level is relatively high. Though the most accurate data will tend to be located around the zero point, i.e. the point $t = 0$, which was used to generate the polynomial expansion. If the subsequent harmonic analysis concentrates on a few cycles of the harmonic signal generated about the point $t = 0$, a few cycles of a harmonic signal that is very is close in value to the corresponding noise free harmonic function is obtained. We have investigated the effectiveness of the technique with a simulated exponential function using normally disctributed noise with a mean of 0.0 (units) and a range of values for the standard deviation. In figure (1a) 25 data points were used. In figures(3a), (4a) and (5a) 250 data points were used. In general for a given noise level the quality of the functions that are generated by the processes that we describe in this article tends to improve with the number of data points of the input exponential function that are used to generate harmonic functions.

Discussion

A simple technique that is based on properties connected to the power series of harmonic functions and exponential functions has been developed. It can be used as a basis for relating an exponential function with a particular decay constant to an odd (sinusoidal) and an even (cosinusoidal) function with a corresponding frequency of oscillation. In general it may be unrealistic to obtain more than a fraction of a cycle of these harmonic signals with this approach. In order to obtain more than a full cycle of a harmonic signal we can avail ourselves of the standard trigonometric identities for the cosines and the sines of the sum of two angles (16) and (17). This enables us to combine the harmonic signal that was generated from the exponential signal with cosine and sine functions with a frequency of oscillation that goes through one or more cycles over the time interval for which data was collected. If the frequency of oscillation of the high frequency component is chosen appropriately this process should enable us to obtain several cycles of oscillation of the harmonic signal that results from this process. In particular if the exponential signal is not noise free, this should enable us to obtain several cycles of harmonic signal that are not overwhelmed by the noise that was present in the exponentia data. From our earlier analysis it appears that the harmonic component that is due to the exponential signal tends to be close in value to the harmonic signal that would be obtained from noise

free data for points that are not too distant from the point about which the polynomial expansion was generated, ($t = 0$), in this example. This is useful as it can be used as a basis for further analysis to establish the frequency of oscillation of the resulting harmonic signal. We have thus demonstrated the feasibility of generating harmonic signals from exponential signals. This process can be used to analyse and characterise small sections of truncated exponential signals, without having to wait for the signal to decay down to its tail region, which is the convetional way of collecting data from a signal consisting of an exponential component and noise, e.g when analysing decay constants from an NMR analysis. If some information is available on the nature of the noise that is likely to be present with the desired signal, this process allows simulations to be performed to assess issues such as: the number of data points required; the spacing of data points; the quality of the signal over a particular time interval; the impact of noise on the exponential data on the harmonic signal(s) that are generated from this process; a false alarm analysis to estimate the probability of making a reasonable estimate of the decay constant for a particular noise type and noise intensity.

This approach can be generalised in a number of ways. We have focused on truncated exponential functions in noisy environments in this article. In principle this approach can be extended to look at signals with contributions from several exponential functions. This is significant as it may enable us to improve on the resolution limits suggested by Istratov and Vyvenko (1999), for signals that contain more than one exponential function.

We can exploit the properties of Chebyshev polynomials to integrate the time series. This allows us to obtain an analytic expression for the time series along with a constant of integration. Integration of a Chebyshev series can improve the signal to noise ratio of the Chebyshev expansion of the underlying functions, Fox and Parker (1968), Press et al (1992). Integration is also a useful means of changing the relative intensities of the component exponential signals.

Another generalisation that is important to be aware of is that a signal that is composed of one or more exponential functions and noise can be used to generate two signals, one composed of sinh functions and noise, and the other composed of cosh functions and noise. This may prove to be beneficial as these functions have useful mathematical identies that may be exploited when attempting to characterise the exponential functions in the data set, e.g.

$$\sinh([\Omega \pm \alpha]x) \equiv \sinh(\Omega x)\cosh(\alpha x) \pm \cosh(\Omega)\sinh(\alpha x) \tag{19}$$

$$\cosh([\Omega \mp \alpha]x) \equiv \cosh(\Omega x)\cosh(\alpha x) \mp \sinh(\Omega)\sinh(\alpha x) \tag{20}$$

They can be used as an alternative to generating the harmonic functions from the exponential functions. If this route is taken, the sinh component generates the sinusoidal signals, and the cosh component generates the cosinusoidal component of the harmonic signal.

Use of polynomials, e.g. splines, and Chebyshev polynomials to approximate functions has certain advantages that prove to beneficial for analysing certain types of signals. They generate an analytic approximation to the function of interest. This may be integrated, and if appropriate it may be differentiated as well, (differentiation tends to be noisier than integration). These processes allow the relative intensitites of component signals to be altered, this may help to find a component with a small amplitude, and a small decay constant. It also facilitates the generation of signals with a large number of points. This does not violate information theory. Using polynomial interpolation to estimate the value of the signal at points other than those at which it was estimated will of course in general, produce an error at the points in time where information is required if a measurement was not made at the point(s) of interest. Thus a high density set of estimates of a quantity of interest, that was obtained from a sparse set of measurements will tend to be much noisier than a set of real measurements of a signal that were made at all of the time points of interest.

Another point of interest with regards to integration is that harmonic signals can be generated by integration. For example, if the original signal had the form

$$s(t) = A\ \cos(\alpha x) + n(t) \tag{21}$$

Integrating this signal results in a signal of the form

$$s'(t) = \frac{A\ \sin(\alpha x)}{\alpha} + n'(t) \tag{22}$$

It may be possible to utilise one or both of expressions (17), and (18)to generate a harmonic function that oscillates over several cycles for a time

interval over which the data has been collected. This signal can in principle be analysed by standard Fourier techniques. It has the form

$$s''(t) = A'' \cos(\Omega x + \alpha x) + n''(t) \tag{23}$$

A similar approach will apply to the signal

$$\widehat{s(t)} = A \ \sin(\alpha x) + n(t) \tag{24}$$

It is important to mention the Bayesian approach to analysing signals consisting of one or more exponential, most authors discuss the resolution constraints that are associated with this method, e.g. Ruanaidh and Fitzgerald, (1996). This approach is useful as it comes with an in built statistical analysis as a means of quality control. In principle it should be possible to combine a Bayesian approach with the above approach to analyse how this technique responds to the type of noise that is expected to be associated with the measurements, or alternaively to estimate the properties of the noise that are associated with a set of measurements.

A simple alternative to this is to undertake a false alarm analysis by performing a large number of simulations on data that corresponds to the expected signal, and the noise that is expected to be associated with a set measurements. This should enable an estimate to be made of the fitness for a particular purpose of this technique, for a data set of interest.

Conclusion

We have developed a simple technique that uses elementary mathematics, the power series of exponential, cosine and sine functions, standar trigonometric identities and, and basic polynomial interpolation theory. This approach is simple to implement and it is also straight forward to test it for fitness for the intended purpose. We have also used elementary trigonometry to derive simple expressions that may enable the analysis and characterisation of a fraction of a sinusoidal function. This is potentially of great value, in particular when dealing with harmonic functions with a small circular frequency relative to the time over which it is possible to collect the data that generates the harmonic functions. It follows this work may be of value if it is necessary to analyse a data set that may contain a truncated exponential function. This facility allows the user to concentrate on the high signal to

noise end of the data set and it may also result in a significant time saving if the decay constant is small. This work also has the potential to be extended so that it can be applied to analyse data sets that consist of more than one exponential function. This may result in a simple approach to analysing a problem that arises in a wide range of experimental techniques.

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Figure captions

Figure 1a

This graph consists of 25 evenly spaced data points over the time interval, $-1 \leq t \leq 1$. It is a graph of the exponential function, $s(t) = e^{-t}$

Figure 1b

This graph is the graph of the sinusoidal function that is generated from the odd component of the power series of the exponential function.

Figure 1c

This graph is the graph of the sinusoidal function that is generated from the even component of the power series of the exponential function.

Figure 1d

This graph is the graph of the high frequency harmonic function that is generated from the power series of the exponential function. The angular frequency corresponding to $\Omega + \alpha$, is 23.56 s^{-1}.

Figure 2a

This graph consists of 25 evenly spaced data points over the time interval, $-1 \leq t \leq 1$. It is a graph of a signal, s(t) consisting of the exponential function, and a noise term, $n(t)$, $s(t) = e^{-t} + n(t)$. The noise is normally distributed with a mean of 0.0 (Units), and a standard deviation of 0.01 (Units).

Figure 2b

This graph is the graph of the high frequency harmonic function that is generated from the power series of the signal s(t). The angular frequency corresponding to $\Omega + \alpha$, is 23.56 s^{-1}.

Figure 3a

This graph consists of 250 evenly spaced data points over the time interval, $-1 \leq t \leq 1$. It is a graph of a signal, s(t) consistingof the exponential function, and a noise term, $n(t)$, $s(t) = e^{-t} + n(t)$. The noise is normally distributed with a mean of 0.0 (Units), and a standard deviation of 0.05 (units).

Figure 3b

This graph is the graph of the high frequency harmonic function that is generated from the power series of the signal s(t). The angular frequency corresponding to $\Omega + \alpha$, is 23.56 s^{-1}.

Figure 4a

This graph consists of 250 evenly spaced data points over the time interval, $-1 \leq t \leq 1$. It is a graph of a signal, s(t) consistingof the exponential function, and a noise term, $n(t)$, $s(t) = e^{-t} + n(t)$. The noise is normally distributed with a mean of 0.0 (Units), and a standard deviation of 0.1 (units).

Figure 4b

This graph is the graph of the high frequency harmonic function that is generated from the power series of the signal s(t). The angular frequency corresponding to $\Omega + \alpha$, is 23.56 s^{-1}.

Figure 5a

This graph consists of 250 evenly spaced data points over the time interval, $-1 \leq t \leq 1$. It is a graph of a signal, s(t) consistingof the exponential function, and a noise term, $n(t)$, $s(t) = e^{-t} + n(t)$. The noise is normally distributed with a mean of 0.0 (Units), and a standard deviation of 0.5 (units).

Figure 5b

This graph is the graph of the high frequency harmonic function that is generated from the power series of the signal s(t). The angular frequency corresponding to $\Omega + \alpha$, is 23.56 s^{-1}.

Fig (1a)
Noise free decaying exponential

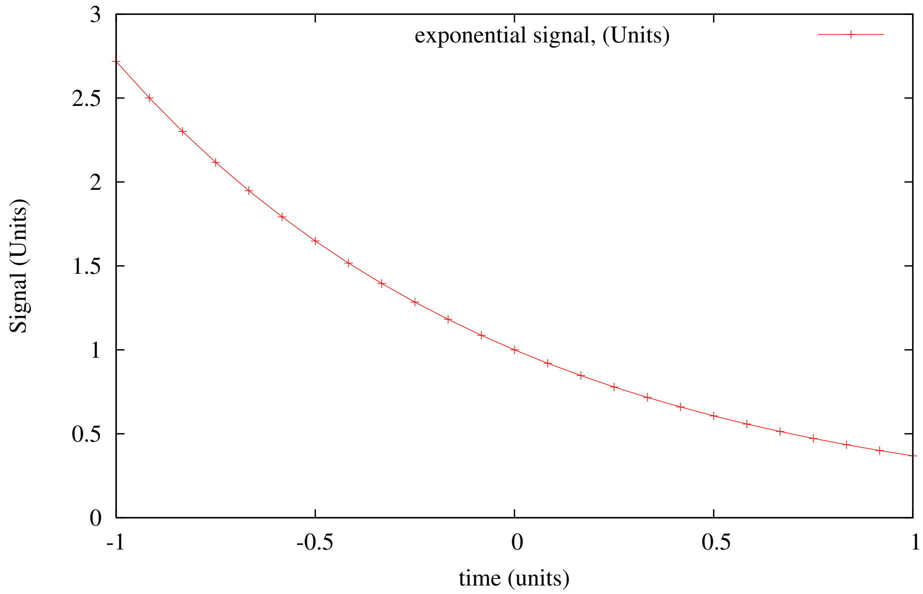

Fig (1b)

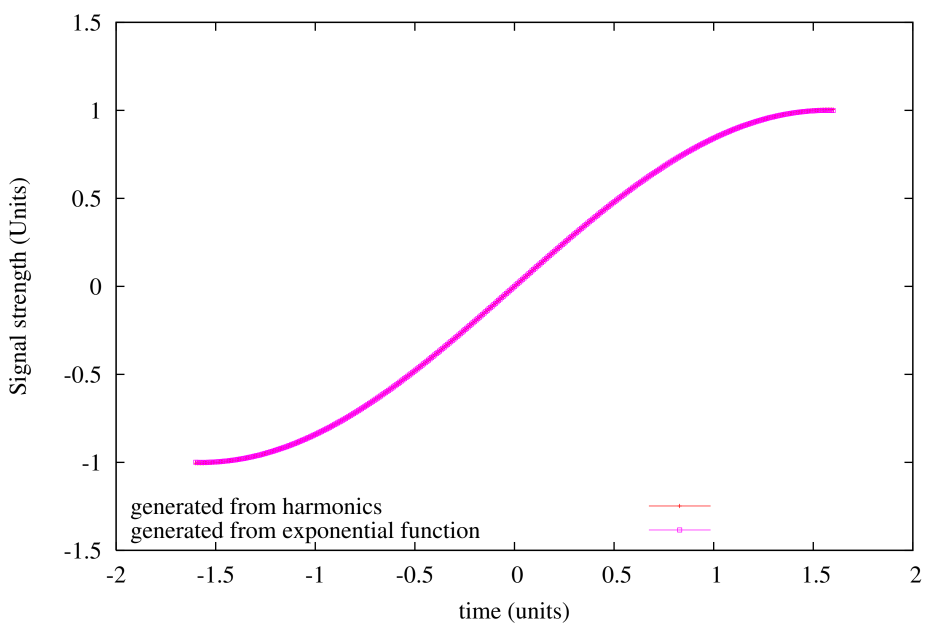

Fig (1c)

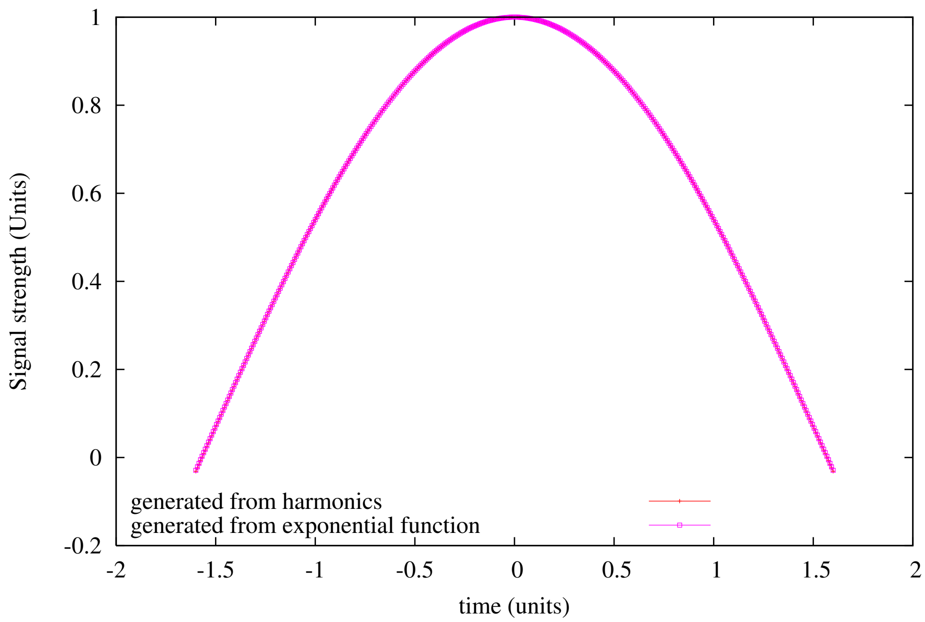
Signal strength (Units)
time (units)
generated from harmonics
generated from exponential function
1
0.8
0.6
0.4
0.2
0
-0.2
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

Fig (1d)

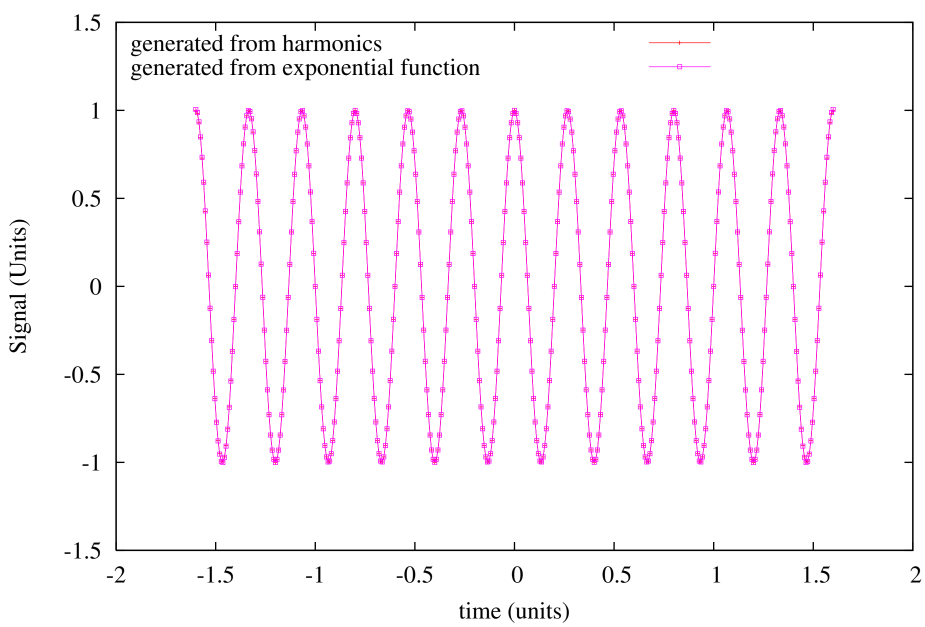
Signal (Units)
time (units)
generated from harmonics
generated from exponential function
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

Fig (2a)
Comparing exponential signals

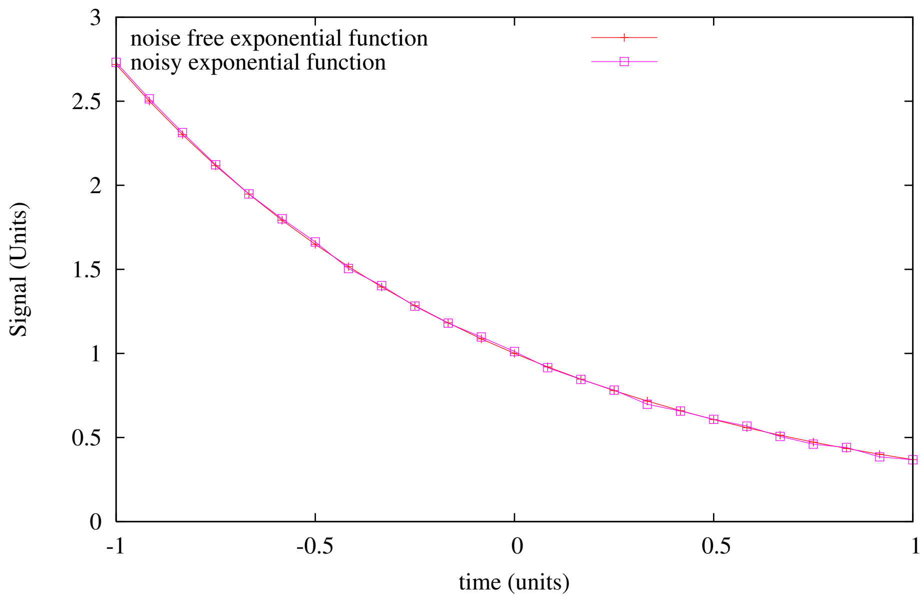

Fig (2b)
Comparing multiple cycle signals

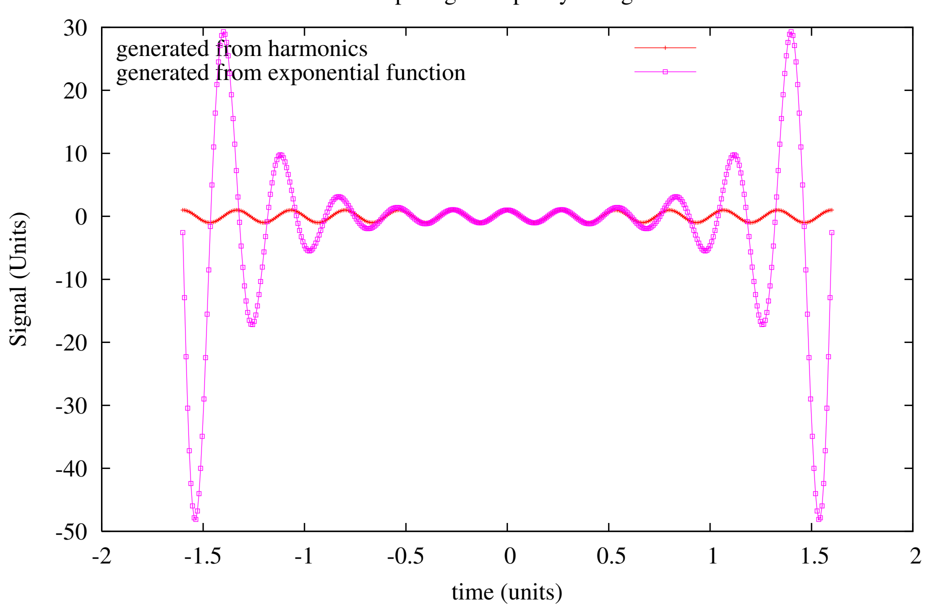

Fig (3a)
Comparing exponential signals

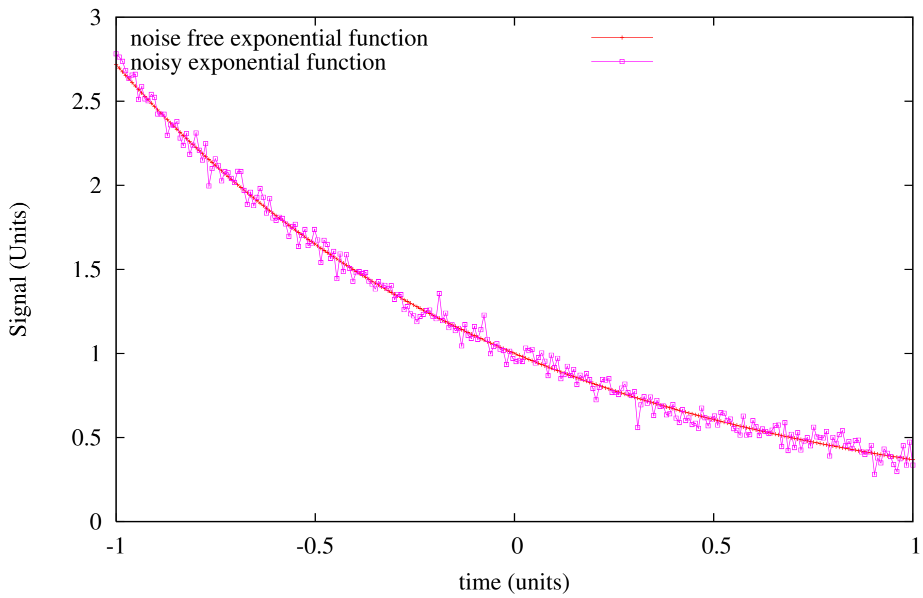

Fig (3b)
Comparing multiple cycle signals

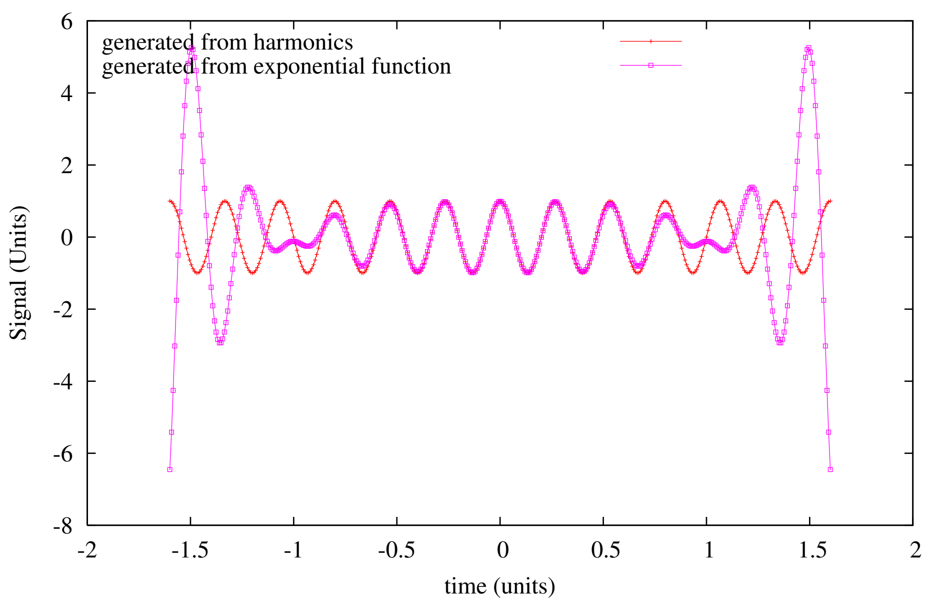

Fig (4a)
Comparing exponential signals

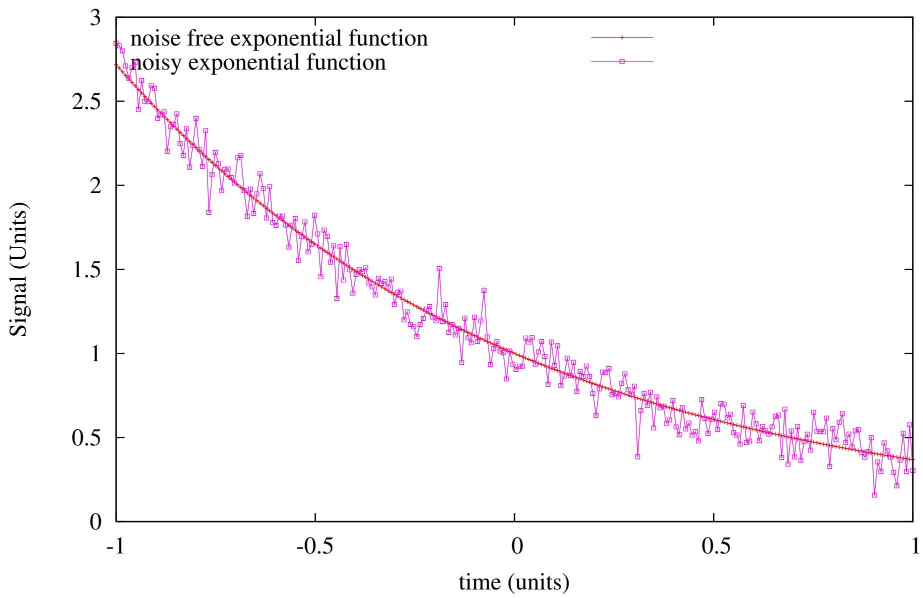

Fig (4b)
Comparing multiple cycle signals

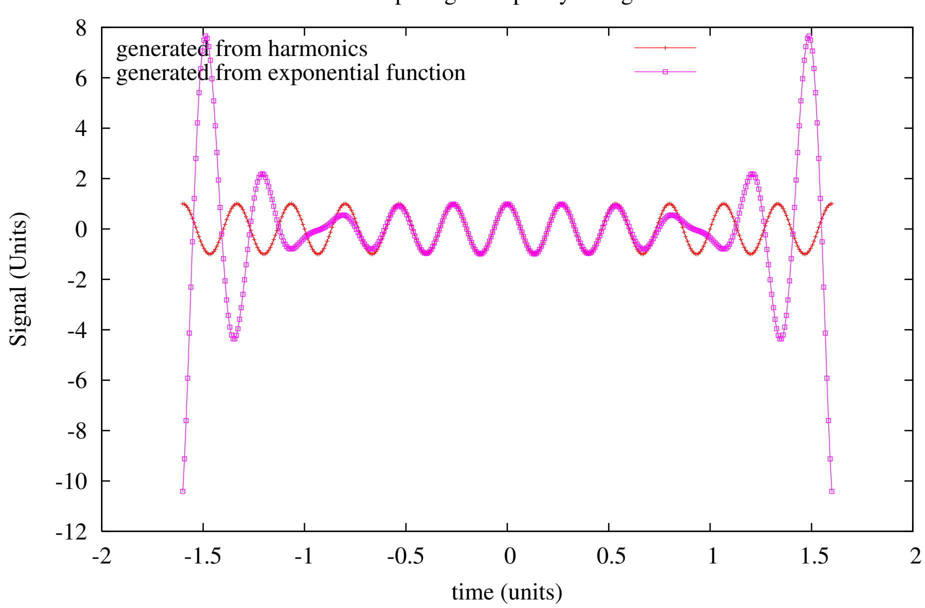

Fig (5a)
Comparing exponential signals

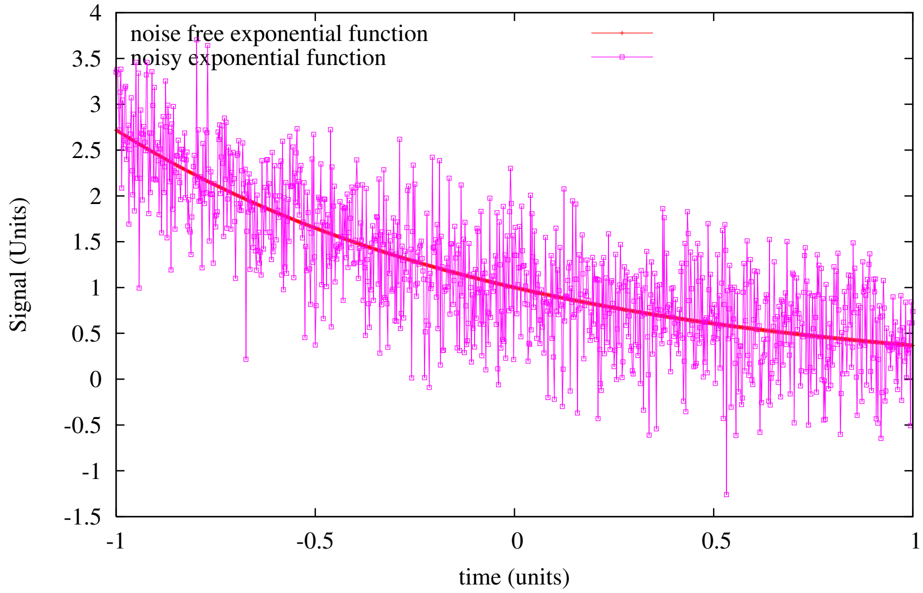

Fig (5b)
Comparing multiple cycle signals